## **WEST Search History**

Hide Items Restore Clear Cancel

DATE: Monday, September 25, 2006

Hide? Set Name Query			Hit Count	
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П	T 1	(dicatioic diarylfuran) clm	0	

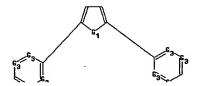
END OF SEARCH HISTORY

## 10721,525

FILE 'HOME' ENTERED AT 13:03:45 ON 25 SEP 2006

=> file reg

=>Uploading C:\Program Files\Stnexp\Queries\10721525a.str



15 15

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

chain bonds : 5-8 11-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11 12-13 12-17 13-14 14-

15 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-8 7-8 7-11 8-9 9-10 10-11 11-14 12-13 12-17

13-14 14-15 15-16 16-17

isolated ring systems :

containing 1 : 7 : 12 :

G1:0,S,N

G2:0,S,N

G3:C,O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L1 STRUCTURE UPLOADED

=> dis 11

L1 HAS NO ANSWERS

L1 STR

Structure attributes must be viewed using STN Express query preparation.

```
=> s 11 sam
              O SEA SSS SAM L1
L2
=> s l1 full
              6 SEA SSS FUL L1
L3
=> file caplus
=> s 13
L4
             6 L3
=> s 14 and pd< nov 2002
      22740598 PD< NOV 2002
                 (PD<20021100)
             4 L4 AND PD< NOV 2002
L5
=> dis 15 1-4 bib abs hitstr
     ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
L5
     2000:790486 CAPLUS Full-text
AN
DN
     133:335249
     Preparation of pesticidal triazine derivatives
TI
     Steiger, Arthur; Zambach, Werner; Jeanguenat, Andre; Eberle, Martin; Trah,
IN
     Stephan; Farooq, Saleem
     Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft
PA
     m.b.H.
so
     PCT Int. Appl., 101 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                           APPLICATION NO.
                                                                   DATE
                                            -----
PΙ
     WO 2000066568
                         A1
                                20001109
                                           WO 2000-EP3921
                                                                   20000502 <--
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
             CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
             ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
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LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

## 10721,525

RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG 20001109 CA 2000-2368582 20000502 <--CA 2368582 AA EP 2000-922671 20000502 <--EP 1175410 **A1** 20020130 EP 1175410 **B**1 20051207 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY BR 2000010294 Α 20020213 BR 2000-10294 20000502 <--JP 2002543191 T2 20021217 JP 2000-615599 20000502 AU 762755 B2 20030703 AU 2000-42986 20000502 RU 2252217 C2 20050520 RU 2001-132322 20000502 AT 312085 Е 20051215 AT 2000-922671 20000502 Т3 ES 2000-922671 ES 2254165 20060616 20000502 ZA 2001008943 Α 20020625 ZA 2001-8943 20011030 <--20030220 US 2001-6954 20011205 US 2003036544 A1 US 6723720 B2 20040420 PRAI CH 1999-832 19990504 Α WO 2000-EP3921 W 20000502 MARPAT 133:335249 OS GI

$$X^{1}$$
 $N-N$ 
 $R^{2}$ 
 $N-R^{1}$ 
 $X^{2}$ 
 $X^{2}$ 
 $X^{2}$ 
 $X^{3}$ 
 $X^{2}$ 
 $X^{3}$ 
 $X^{4}$ 
 $X^{5}$ 
 $X^{5$ 

The title compds. [I; R1 = (un) substituted aryl, heteroaryl; R2 = H, OH, halo, etc.; A = a single bond, alkylene, O, O(alkylene); X1 = halo, CN, NO2, etc.; X2, X3 = H, halo, CN, etc.] which are suitable especially in the control of pests in agriculture and stored goods and also in the keeping of domestic animals, were prepared Thus, treatment of 2,6- difluoroacetophenone with Br2 in the presence of AlCl3 in CHCl3 followed by reaction of the resulting 2-bromo-1-(2,6-difluorophenyl)ethanone with 4-bromobenzoic acid hydrazide in the presence of AgOAc in dimethoxyethane afforded triazine II. Biol. data for compds. I was given.

IT 304671-84-9P 304671-86-1P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of pesticidal triazine derivs.)

RN 304671-84-9 CAPLUS

CN 1,2,4-Triazine, 3-(2,6-difluorophenyl)-6-[5-[4-(trifluoromethyl)phenyl]-2-thienyl]- (9CI) (CA INDEX NAME)

RN 304671-86-1 CAPLUS

CN 1,2,4-Triazine, 3-(2,6-difluorophenyl)-6-[5-[4-(trifluoromethoxy)phenyl]-2-thienyl]- (9CI) (CA INDEX NAME)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1990:235248 CAPLUS Full-text

DN 112:235248

TI 1,4-Bis(3-oxo-2,3-dihydropyridazin-6-yl)benzene analogs: potent phosphodiesterase inhibitors and inodilators

AU Coates, William J.; Prain, H. Douglas; Reeves, Martin L.; Warrington, Brian H.

CS Smith Kline and French Res. Ltd., Welwyn/Hertfordshire, AL6 9AR, UK

SO Journal of Medicinal Chemistry (1990), 33(6), 1735-41 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CASREACT 112:235248

GΙ

$$\begin{bmatrix} 0 & & & \\$$

AB The title compds. I (R = H, Me; X = S, CH2; Z = 1,4-, 1,3-C6H4, 2,5-thienyl, 4-C6H4C6H4-4') were prepared from bis(alkanoyl) benzenes by conversion to γ-keto acids and treatment with N2H4. I were evaluated for inhibition of low Km, cAMP-selective, cGMP-inhibited phosophodiesterase (PDE III) and hemodynamic activity. The most potent PDE III inhibitor was I (R = Me, X = CH2, Z = 1,4-C6H4) which also retained the greatest inotropic and vasodilator potency. PDE III inhibitory potency is associated with overall planar topol. of the phenylpyridazinone moiety and the presence of two critically separated electroneg. centers. The generally higher level of PDE III inhibitory potency of I relative to 6-(4-substituted-phenyl)pyridazin-3(2H)-one derivs. (e.g. Sicar, I; et al., 1987, Moos, W.H.; et al., 1987) derives from a closer to optimal separation of two interacting points in the inhibitor mol. achieved through the more extended bis(azinone) structure. Correlation between the

pharmacol. and PDE III inhibitory activities of I provides addnl. evidence for PDE III being an important mediator of inodilator action.

IT 112127-79-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, ionotropic, vasodilator, and phosphodiesterase inhibiting activities of)

RN 112127-79-4 CAPLUS

CN 3(2H)-Pyridazinone, 6,6'-(2,5-thiophenediyl)bis- (9CI) (CA INDEX NAME)

L5 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1988:48712 CAPLUS Full-text

DN 108:48712

TI Strategic approaches to drug design. II. Modeling studies on phosphodiesterase substrates and inhibitors

AU Davis, A.; Warrington, B. H.; Vinter, J. G.

CS Smith Kline and French Res., Welwyn/Herts., AL6 9AR, UK

SO Journal of Computer-Aided Molecular Design (1987), 1(2), 97-119 CODEN: JCADEQ; ISSN: 0920-654X

DT Journal

LA English

AB Computational chem. and mol. graphics were combined with both phys. and biol. data to study the interactions of the cat ventricle phosphodiesterase enzyme with the natural substrates cAMP and cGMP and synthetic inhibitors. Specific binding points (defined by points at which the electrostatic interaction of a proton with the target are most stable) were used to give a consistent picture of the binding requirements of both nonspecific and specific inhibitors. These points are situated on or beyond the van der Waals surface and broadly consist of: (a) a single, large point corresponding with an anionic group and probably representing a primary link; (b) a variable set of points associated with the purine of the natural substrate which are likely to represent the secondary binding area and which are able, in appropriate combination with (a), to define specificity; and (c) a 3rd point which (by hydrophobic interaction) can further affect potency by its (chiral) influence. The complementary study by lone-pair construction and regression anal. reached essentially the same working rules for structure-activity and provided quant. support for the hypothesis. It is notable that structural overlay in this particular case seems to be of less significance than electronic overlay. Indeed, structural comparisons have been misleading at times. The main driving forces for recognition and orientation are undoubtedly the coulombic interactions which were the subject of these studies. However, steric influences play their part in the bound state. Compds. designed to access the more effective N(1) site demonstrated by these studies were found to show the expected high potency.

IT 112127-79-4

RL: BIOL (Biological study)

(cyclic nucleotide phosphodiesterase inhibition by, structure in relation to)

RN 112127-79-4 CAPLUS

CN 3(2H)-Pyridazinone, 6,6'-(2,5-thiophenediyl)bis- (9CI) (CA INDEX NAME)

L5 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1977:165774 CAPLUS Full-text

DN 86:165774

TI Effect of arylfuran derivatives on the activity of pyridoxal enzymes

AU Fadeeva, N. I.; Gus'kova, T. A.; Pershin, G. N.; Degtyareva, I. N.

CS Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR

SO Khimiko-Farmatsevticheskii Zhurnal (1976), 10(12), 21-6 CODEN: KHFZAN; ISSN: 0023-1134

DT Journal

LA Russian

GI

Of 27 arylfuran derivs. tested, 5-(p-chlorophenyl)-2-bromoacetylfuran (I) [39170-34-8] was the most active antimicrobial agent against common bacterial and fungal species in vitro and the strongest inhibitor of aspartate aminotransferase (EC 2.6.1.1) (AST) [9000-97-9] and alanine aminotransferase (EC 2.6.1.2) (ALT) [9000-86-6]. Its p-nitro analog [39170-35-9] did not inhibit the pyridoxal enzymes and showed only weak bacteriostatic and fungistatic activities. 5-(P-bromophenyl)furyl-2- glyoxal [42142-86-9] showed strong antimicrobial and AST-inhibitory activities but did not inhibit ALT. Mercapto-containing arylfurans showed weak enzyme-inhibitory and antimicrobial activities, but thiazole, pyrrocoline, and imidazopyridine derivs. were inactive. Some of the 5-aryl-2-bromobutyl (propionyl) furan derivs. showed weak antimicrobial activity but did not affect the pyridoxal enzymes, suggesting an effect on other enzymic systems. Use of the aminotransferases is suggested in primary screening of arylfuran compds. for antimicrobial activity.

IT 62530-40-9

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(bactericidal and fungicidal activities of, aminotransferase activity in relation to)

RN 62530-40-9 CAPLUS

CN 1,2,4-Triazin-3(2H)-one, 6-[5-(4-bromophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)

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=> s 14 not 15
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L6 2 L4 NOT L5

=> dis 1-2 bib abs

- L6 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2006:163781 CAPLUS Full-text
- DN 144:400522
- TI Synthesis and characterization of new fluorescent two-photon absorption chromophores
- AU Huang, Ping-Hsin; Shen, Jiun-Yi; Pu, Shin-Chien; Wen, Yuh-Sheng; Lin, Jiann T.; Chou, Pi-Tai; Yeh, Ming-Chang P.
- CS Institute of Chemistry, Academia Sinica, Taipei, Taiwan
- SO Journal of Materials Chemistry (2006), 16(9), 850-857 CODEN: JMACEP; ISSN: 0959-9428
- PB Royal Society of Chemistry
- DT Journal
- LA English
- Dipolar and quadrupolar type two-photon absorption (TPA) compds. were synthesized and TPA cross sections ( $\sigma$ ) were measured by Ti:sapphire femtosecond laser excitation fluorescence ( $\lambda$  = 800 nm). Among them, [2,5-bis-[5-(4-diphenylaminophenylethynyl)thiophen-2-yl]- [1,3,4]oxadiazole], 12, was structurally characterized by x-ray crystallog. The resulting data indicate that the structure of this compound possesses excellent coplanarity. The compds. have arylamines as the donor, and [1,3,4]oxadiazolyl, cyanovinyl or pyridazin-3,6-diyl moiety as the acceptor. Variation of arylamines and pendant alkyl groups has a significant influence on  $\sigma$  values. By an appropriate combination of donor and acceptor,  $\sigma$  values of > 103 GM (10-50 cm4s photon·mol.-1) can be achieved. One quadrupolar mol. (13) possessing an arylamine donor and a pyridazine acceptor has both a high  $\sigma$  value (1442 GM) and  $\sigma$ /MW (1.97 GM/q).
- RE.CNT 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2004:38041 CAPLUS Full-text
- DN 141:260474
- TI Synthesis and biological activity of thiophene derivatives
- AU Shklyaev, Yu. V.
- CS Inst. Tekh. Khim., Ural. Otd., RAN, Perm, 614990, Russia
- SO Kislorod- i Serusoderzhashchie Geterotsikly, [Trudy Mezhdunarodnoi Konferentsii "Khimiya i Biologicheskaya Aktivnost Kislorod- i Serusoderzhashchikh Geterotsiklov"], 2nd, Moscow, Russian Federation, Oct. 14-17, 2003 (2003), Volume 1, 472-477. Editor(s): Kartsev, Viktor G. Publisher: IBS Press, Moscow, Russia. CODEN: 69EZN9; ISBN: 5-902545-01-3
- DT Conference
- LA Russian
- OS CASREACT 141:260474
- AB A series of 2-thienylglyoxylic esters RCOCO2Et (R = substituted 2-thienyl) was synthesized by either Friedel-Crafts acylation of thiophenes with Et oxalyl chloride or reaction of thiophene Grignard reagents with di-Et oxalate. The antimicrobial activity of thiosemicarbazones of these esters and of trimethylammonium-functionalized hydrazides of acetyl thiophenes was studied.

## 10721,525

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	28.33	195.48
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.50	-4.50

STN INTERNATIONAL LOGOFF AT 13:05:12 ON 25 SEP 2006